

#Ligand	TotalEnergy	VDW	AverConPair
7khp-Roccustyrna_fr1-0.pdb	-955.241	-955.241	107.536
7khp-Roccustyrna_fr2-0.pdb	-100.469	-100.469	195.152
7khp-Roccustyrna_fr3-0.pdb	285.525	285.525	830.769
7khp-Roccustyrna_fr4-0.pdb	-784.913	-784.913	167.222
7khp-Roccustyrna_fr5-0.pdb	277.179	277.179	790.196
7khp-Roccustyrna_fr6-0.pdb	-858.212	-858.212	199.737
7khp-Roccustyrna_fr7-0.pdb	-879.123	-879.123	184.571
7khp-Zanamivir_CID_60855-0.pdb	-686.283	-686.283	212.609
7khp-Vidarabine_CID_21704-0.pdb	-794.631	-794.631	261.053
7khp-Valganciclovir_CID_135413535-0.pdb	752.042	752.042	16.92
7khp-Tenofovir_CID_464205-0.pdb	-638.048	-638.048	208.947
7khp-Taribavirin_CID_451448-0.pdb	-667.285	-667.285	235.882
7khp-Sorivudine_CID_5282192-0.pdb	-232.063	-232.063	17.35
7khp-Sofosbuvir_CID_45375808-0.pdb	149.669	149.669	160.278
7khp-Ritonavir_CID_392622-0.pdb	185.555	185.555	8.98
7khp-Penciclovir_CID_135398748-0.pdb	-821.633	-821.633	293.333
7khp-Nelfinavir_CID_64143-0.pdb	273.185	273.185	13.95
7khp-Merimepodib_CID_153241-0.pdb	-89.827	-89.827	186.061
7khp-Maribavir_CID_471161-0.pdb	-910.169	-910.169	255.417
7khp-Lopinavir_CID_92727-0.pdb	234.093	234.093	150.217
7khp-Indinavir_CID_5362440-0.pdb	-869.632	-869.632	130.444
7khp-Inarigivir_CID_6912016-0.pdb	-945.278	-945.278	199.487
7khp-Galidesivir_CID_10445549-0.pdb	-68.937	-68.937	257.368
7khp-Famciclovir_CID_3324-0.pdb	351.937	351.937	206.957
7khp-Faldaprevir_CID_42601552-0.pdb	328.375	328.375	130.877
7khp-Darunavir_CID_213039-0.pdb	-843.131	-843.131	159.737
7khp-Cytarabine_CID_6253-0.pdb	-688.448	-688.448	280.588
7khp-Boceprevir_CID_10324367-0.pdb	289.311	289.311	193.243
7khp-Atazanavir_CID_148192-0.pdb	136.918	136.918	149.804
7khp-Asunaprevir_CID_16076883-0.pdb	-739.324	-739.324	129.412
7khp-Amprenavir_CID_65016-0.pdb	-768.666	-768.666	141.429
7khp-GissitorviffirnaTM1-0.pdb	-673.636	-673.636	221.818
7khp-GissitorviffirnaTM4-0.pdb	-708.798	-708.798	27.45
7khp-GissitorviffirnaTM6-0.pdb	618.408	618.408	277.436
7khp-GissitorviffirnaTM7-0.pdb	-955.275	-955.275	190.789
7khp-GissitorviffirnaTM8-0.pdb	-829.762	-829.762	158.947
7khp-GissitorviffirnaTM9-0.pdb	-937.469	-937.469	176.176
7khp-Roccustyrna_gs1-0.pdb	169.125	169.125	177.391
7khp-Roccustyrna_gs2-0.pdb	-707.819	-707.819	222.632
7khp-Roccustyrna_gs3-0.pdb	585.832	585.832	238.085
7khp-Roccustyrna_gs4-0.pdb	181.467	181.467	852.941
7khp-Roccustyrna_gs5-0.pdb	-354.048	-354.048	754.688
7khp-Roccustyrna_gs6-0.pdb	-735.307	-735.307	23.1
7khp-Roccustyrna_gs8-0.pdb	496.635	496.635	23.54